PFOA

335-67-1 | DTXSID8031865

Model Performance

Ν	Model	Data

Weighted KNN model

5-fold C\	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 4.17

Global applicability domain: Inside

Local applicability domain index: 9.71e-01

Confidence level: 6.82e-01

Nearest Neighbors from the Training Set

Image not found

Butylamine

Measured: 3.61 Predicted: 4.09 Image not found

Isopentyl alcohol

Measured: 4.52 Predicted: 4.24 Image not found

Pyrrolidine

Measured: 4.07 Predicted: 4.10

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1-Butanol

Measured: 4.19 Predicted: 4.03

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1-Pentanol

Measured: 4.69 Predicted: 4.17